

Outer-Product-Free Sets for Polynomial Optimization and Oracle-Based Cuts

Daniel Bienstock, Chen Chen, Gonzalo Muñoz

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Abstract

Cutting planes are derived from specific problem structures, such as a single linear constraint from an integer program. This paper introduces cuts that involve minimal structural assumptions, enabling the generation of strong polyhedral relaxations for a broad class of problems. We consider valid inequalities for the set $S \cap P$, where S is a closed set, and P is a polyhedron. Given an oracle that provides the distance from a point to S we construct a pure cutting plane algorithm; if the initial relaxation is a polytope, the algorithm is shown to converge. Cuts are generated from convex forbidden zones, or S -free sets derived from the oracle. We also consider the special case of polynomial optimization. Polynomial optimization may be represented using a symmetric matrix of variables, and in this lifted representation we can let S be the set of matrices that are real, symmetric outer products. Accordingly we develop a theory of *outer-product-free* sets. All maximal outer-product-free sets of full dimension are shown to be convex cones and we identify two families of such sets. These families can be used to generate intersection cuts that can separate any infeasible extreme point of a linear programming relaxation in polynomial time. Moreover, in the special case of polynomial optimization we derive strengthened oracle-based intersection cuts that can also ensure separation in polynomial time.

1 Introduction

Consider a generic mathematical program of the following form

$$\begin{aligned} & \min c^T x \\ & \text{subject to } x \in S \cap P. \end{aligned}$$

$P := \{x \in \mathbb{R}^n | Ax \leq b\}$ is a polyhedral set, the objective function is linear with coefficients $c \in \mathbb{R}^n$, and $S \subset \mathbb{R}^n$ is a closed set. This paper concerns the construction of linear programming relaxations of the form $\min c^T x | x \in P_0$ with some polyhedron P_0 defining the relaxed feasible region, $P_0 \supseteq S \cap P$. A natural choice of relaxation is to set $P_0 := P$; however, this may be a poor approximation of the original problem. This paper focuses focus on the issue of an inexact relaxation in which P_0 has at least one extreme point \bar{x} that is not in $P \cap S$. Our remedy is to repeatedly augment P_0 with a cut: a halfspace H such that $H \supseteq S \cap P$ and removing some portion of P_0 . This is done recursively via a cutting plane algorithm: first generating a set of cuts V_0 for P_0 , then deriving cuts V_1 for $P_1 := V_0 \cap P$, and so forth. As the relaxed feasible regions P_0, P_1, \dots, P_k are

polyhedra, the associated relaxations can all be solved efficiently with linear programming (as long as P_0 and the cuts are described with rational data), providing iteratively tighter dual bounds for the original problem. Cutting planes are crucial to branch-and-cut methods (e.g. [7, 19, 62, 66, 79]) for global optimization.

There are many ways to generate cuts such as: disjunctions [10], lift-and-project [56], algebraic arguments (e.g. [6, 40, 42, 59]), combinatorics (see [82]), and convex outer-approximation (e.g. [46]). We adopt the geometric perspective, in which cuts are derived from convex forbidden zones, or S -free sets. The convexity requirement on S -free sets is essential in the generation of intersection cuts, although nonconvex forbidden zones with special structure could also be used to generate cuts (e.g. cross cuts [52]). Cutting plane generation depends on the specific structure of S and P , such as $S = \mathbb{Z}^n$ in the case of pure integer programming. We present computationally efficient cuts with minimal structural assumptions. Suppose there is an oracle that provides the distance from a point to S . This distance can be approximated to arbitrary accuracy in the case of integer programming (using rounding operations) and polynomial optimization (using eigenvalues, see Section 3). Theorem 3.3 establishes that, given the initial relaxation P_0 is a polytope, this oracle (or an arbitrarily close approximation thereof) enables a finite-time cutting plane algorithm that constructs a polyhedron arbitrarily close to $\text{conv}S \cap P$. Hence an explicit functional characterization of S is not necessary to produce a strong relaxation.

We also consider a more specific problem, polynomial optimization (aka polynomial programming):

$$\begin{aligned} & \min p_0(x) \\ (\mathbf{PO}) \quad & \text{s.t. } p_i(x) \leq 0 \quad i = 1, \dots, m. \end{aligned}$$

Each p_k is a polynomial function with respect to the decision vector $x \in \mathbb{R}^n$. Polynomial optimization generalizes important classes of problems such as quadratic programming, and has numerous applications in engineering; moreover, the quadratic representation of binary variables can also be useful for generating strong relaxations of discrete problems (e.g. MAXCUT [39]). We work with a representation of \mathbf{PO} that uses a symmetric matrix of decision variables, and let S be the set of symmetric matrices that can be represented as a real, symmetric outer product — accordingly we study *outer-product-free* sets. Two families of full-dimensional maximal outer-product-free sets are identified in Theorems 4.9 and 4.12, which characterize all such sets in the space of 2×2 symmetric real matrices. We derive cuts from these outer-product-free sets using the intersection cut [9], which enables separation of any infeasible extreme point of a (lifted) polyhedral relaxation of \mathbf{PO} in polynomial time.

In global optimization, cuts typically rely on particular substructures (see e.g. [45]) and target single terms or functions to derive cuts [15, 53, 57, 61, 70, 76–78]. In contrast we develop cuts that can account for all variables of the problem simultaneously. To the best of our knowledge there are two papers that are similar in this regard. The disjunctive cuts of Saxena, Bonami, and Lee [71, 72] apply to mixed-integer programming with nonconvex quadratic constraints (MIQCP) with all variables bounded; bounded polynomial optimization problems can be transformed to bounded MIQCP. Their cuts are derived from a mixed-integer linear programming (MILP) approximation of the problem. Ghaddar, Vera, and Anjos [38] propose a lift-and-project method, generating cuts to strengthen a given moment relaxation by separating over a higher-moment relaxation. They show that the method can be interpreted as a generalization of the lift-and-project of Balas, Ceria, and Cornuéjols [11] for mixed-integer linear programming. Polynomial-time separation for their

procedure is not guaranteed in general, but some guarantees regarding separation and convergence can be made in the special case of nonnegative variables and in the case of binary variables.

1.1 Notation

Denote the interior of a set $\text{int}(\cdot)$ and its boundary $\text{bd}(\cdot)$. The convex hull of a set is denoted $\text{conv}(\cdot)$, and its closure is $\text{clconv}(\cdot)$; likewise, the conic hull of a set is $\text{cone}(\cdot)$, and its closure $\text{clcone}(\cdot)$. The set of extreme points of a convex set is $\text{ext}(\cdot)$. For a point x and nonempty set S in \mathbb{R}^n , we define $d(x, S) := \inf_{s \in S} \{\|x - s\|_2\}$; note that for S closed we can replace the infimum with minimum. Denote the ball with center x and radius r to be $\mathcal{B}(x, r)$. For a square matrix X , $X_{[i,j]}$ denotes the 2×2 principal submatrix induced by indices $i \neq j$. $\langle \cdot, \cdot \rangle$ denotes the matrix inner product. A positive semidefinite matrix may be referred to as a PSD matrix for short, and likewise NSD refers to negative semidefinite.

The remainder of the paper is organized as follows. Section 2 describes S -free sets, the intersection cut, and a cut strengthening procedure. Section 3 develops the oracle-based cut. Section 4 studies outer-product-free sets. Section 5 describes cut generation using outer-product-free sets. Section 6 offers numerical examples. Section 7 concludes.

2 S -free Sets and the Intersection Cut

2.1 S -Free Sets

Definition 2.1. A set $C \subset \mathbb{R}^n$ is S -free if $\text{int}(C) \cap S = \emptyset$ and C is convex.

For any S -free set C we have $S \cap P \subseteq \text{clconv}(S \setminus \text{int}(C))$, and so any valid inequalities for $\text{clconv}(S \setminus \text{int}(C))$ are valid for $S \cap P$. Larger S -free sets can be useful for generating deeper cuts [25].

Definition 2.2. An S -free set C is *maximal* if $V \not\supset C$ for all S -free V .

Under certain conditions (see [17, 25, 27, 48]), maximal S -free sets are sufficient to generate all nontrivial cuts for a problem. When $S = \mathbb{Z}^n$, C is called a lattice-free set. Maximal lattice-free sets are well-studied in integer programming theory [4, 5, 16, 22, 31, 42, 48, 55], and the notion of S -free sets was introduced as an extension [32].

So far we have left aside discussion on how precisely one can derive cuts from an S -free set C . Averkov [8] provides theoretical consideration on the matter; for instance, characterizing when $\text{conv}(P \setminus C)$ is a polyhedron. In specific instances, the convex hull of $\text{conv}(P \setminus C)$ can be fully described; for example, Bienstock and Michalka [21] provide a characterization of the convex hull when S is given by the epigraph of a convex function and C is polyhedral or ellipsoidal. A standard procedure for generating cuts (but not necessarily the entire hull) is to find a simplicial cone P' containing P and apply Balas' intersection cut [9] for $P' \setminus C$. We shall adopt this approach, which has been studied in great detail (see [25–27]). The first use of simplicial cones to generate cuts can be attributed to Tuy [80] for minimization of a concave function over a polyhedron; such cuts are named Tuy cuts, concavity cuts, or convexity cuts. The distinction is that Tuy cuts are objective cuts whereas intersection cuts are feasibility cuts. Balas and Margot [13] propose strengthened intersection cuts by using a tighter relaxation of P . Porembski [67, 68] proposes a method for strengthening the Tuy cut by using different conic relaxations.

2.2 The Intersection Cut

Let $P' \supseteq P$ be a simplicial conic relaxation of P : a displaced polyhedral cone with apex \bar{x} and defined by the intersection of n linearly independent halfspaces. Any n linearly independent constraints describing P can be used to define a simplicial conic relaxation; consequently any extreme point of P can be used as the apex of P' . A simplicial cone may be written as follows:

$$P' = \{x | x = \bar{x} + \sum_{j=1}^n \lambda_j r^{(j)}, \lambda \geq 0\}. \quad (1)$$

Each extreme ray is of the form $\bar{x} + \lambda_j r^{(j)}$, where each $r^{(j)} \in \mathbb{R}^n$ is a direction and $\lambda \in \mathbb{R}_+^n$ is a vector of scaling factors.

We shall assume $\bar{x} \notin S$, so that \bar{x} is to be separated from S . So let C be an S -free set with \bar{x} in its interior. Since $\bar{x} \in \text{int}(C)$, there must exist $\lambda > 0$ such that $\bar{x} + \lambda_j r^{(j)} \in \text{int}(C) \forall j$. Also, each extreme ray is either entirely contained in C , i.e. $\bar{x} + \lambda_j r^{(j)} \in \text{int}(C) \forall \lambda_j \geq 0$, or else there is an intersection point with the boundary $\text{bd}(\cdot)$: $\exists \lambda_j^* : \lambda_j^* r^{(j)} \in \text{bd}(C)$. The intersection cut is the halfspace whose boundary contains each intersection point (given by λ_j^*) and that is parallel to all extreme rays $r^{(i)}$ contained in C .

The intersection cut can be described algebraically as follows. For each extreme ray that intersects with $\text{bd}(C)$ we have $(\bar{x}^T + \lambda_j^* (r^{(j)})^T) \pi = \pi_0$ (the intersection point lies on the cut boundary), and for a ray contained in C we have $\pi^T r^{(j)} = 0$ (the cut boundary is parallel to the ray). Define $R := [r^{(1)}, r^{(2)}, \dots, r^{(n)}]^T$. Now construct a vector of coefficients $\beta \in \mathbb{R}^n$ so that if the j th extreme ray intersects with $\text{bd}(C)$, then we set $\beta_j = (\lambda_j^*)^{-1}$, otherwise $\beta_j = 0$. The intersection cut with coefficients $\pi \in \mathbb{R}^n$ and intercept $\pi_0 \in \mathbb{R}$ can be derived from the following system of linear equations:

$$[-\beta^T, \beta \bar{x}^T + R] \begin{bmatrix} \pi_0 \\ \pi \end{bmatrix} = 0 \quad (2)$$

Since each intersection point is unique (the extreme rays only intersect at \bar{x}), we are assured of a unique solution up to scaling, i.e. $\dim(\text{null}([-\beta^T, \beta \bar{x}^T + R])) = 1$. If $\beta = 0$, then all extreme rays of P' are contained in C , and we have a certificate of infeasibility of the original problem, as $P \subseteq P' \in \text{int}(C) \implies P \cap S = \emptyset$. Balas [9, Theorem 2] provides a closed-form solution to the coefficients π . Consider P' in inequality form, $P' = \{x | Ax \leq b\}$, where A is a square full rank matrix. Then the coefficients can be expressed as

$$\pi_0 = \sum_{\forall i} (1/\lambda_i^*) b_i - 1, \quad \pi_j = \sum_{\forall i} (1/\lambda_j^*) a_{ij}. \quad (3)$$

Note that the ray indices are assumed to be aligned with the inequality form, i.e. the k th extreme ray is found by setting all but the k th row active. Furthermore, $1/\lambda_j^*$ is treated as zero if the step length is infinite.

Having obtained the hyperplane coefficients π, π_0 we must determine the correct direction of the cut, so let $\beta_0 := \text{sgn}(\pi^T \bar{x} - \pi_0)$, where $\text{sgn}(\cdot)$ denotes the sign function. The intersection cut is:

$$\beta_0 (\pi^T x - \pi_0) \leq 0. \quad (4)$$

Let $V := \{x | \beta_0(\pi^T x - \pi_0) \leq 0\}$ be the halfspace defined by the intersection cut. For completeness we include a proof of validity of V (a fact established in the original paper by Balas [9, Theorem 1]), and furthermore establish a condition in which the cut gives the convex hull of $P' \setminus \text{int}(C)$.

Proposition 2.3. $V \supseteq P' \setminus \text{int}(C)$.

Proof. Suppose by way of contradiction there exists a point $y \in P' \setminus \text{int}(C)$ for which $\beta_0(\pi^T y - \pi_0) > 0$. Since $y \in P'$, then from (1) there exists $\hat{\lambda} \geq 0$ such that $y = \bar{x} + \sum_{j=1}^n \hat{\lambda}_j r^{(j)}$. Furthermore, since $y \notin \text{int}(C)$ there exists some k for which $\hat{\lambda}_k > \lambda_k^*$ where the k th extreme ray intersects with $\text{bd}(C)$. If no such k exists, y may be expressed as the convex combination of points interior to C , and by the convexity of C we have $y \in \text{int}(C)$.

Now from (2) we have that for any extreme ray j of P' contained in C that $\pi^T r^{(j)} = 0$, otherwise $\pi^T(\bar{x} + \lambda_j^* r^{(j)}) = \pi_0 \implies \beta_0 \lambda_j^* \pi^T r^{(j)} \leq \pi_0$. Since $\lambda_j^* > 0$, then $\beta_0 \pi^T r^{(j)} \leq \beta_0 \pi_0$. For the k th extreme ray we have

$$\begin{aligned} \pi^T(\bar{x} + \lambda_k^* r^{(k)}) - \pi_0 &= 0, \\ \implies \beta_0(\pi^T y - \pi_0) &= \beta_0(\pi^T((\hat{\lambda}_k - \lambda_k^*)r^{(k)} + \sum_{j \neq k} \lambda_j r^{(j)})), \\ \implies \beta_0(\pi^T y - \pi_0) &\leq 0. \end{aligned}$$

This contradicts our initial supposition that $\beta_0(\pi^T y - \pi_0) > 0$. \square

Proposition 2.4. Suppose all extreme rays of P' intersect with the boundary of C . Then $\text{clconv}(P' \setminus \text{int}(C)) = P' \cap V$

Proof. From Proposition 2.3 we have $P' \cap V \supseteq P' \setminus \text{int}(C) \implies \text{clconv}(P' \setminus \text{int}(C)) \subseteq P' \cap V$, so only the other direction remains. Suppose there exists $y \in P' \cap V$ such that $y \notin \text{clconv}(P' \setminus \text{int}(C))$, and so $y \in \text{int}(C)$. Now if $y \in \text{bd}(P' \cap V)$, then y is on the boundary of V and so y can be expressed as the convex combination of the intersection points generating the intersection cut. This would imply $y \in \text{clconv}(P' \setminus \text{int}(C))$, so we must assume $y \in \text{int}(P' \cap V)$.

Now consider the ray emanating from \bar{x} and passing through y . Since the ray is contained in P' , which has all its extreme rays intersecting with $\text{bd}(C)$, then by convexity of C it must also intersect with $\text{bd}(C)$. Thus y is on a line segment connecting some point $c \in \text{bd}(C) \cap P'$ and \bar{x} .

Claim. $\bar{x} \notin V$.

Proof: If $\beta_0 = 0$, then $V = \emptyset$. Otherwise, $|\pi^T \bar{x} - \pi_0| > 0$, and so

$$\begin{aligned} \beta_0(\pi^T \bar{x} - \pi_0) &= |\pi^T \bar{x} - \pi_0|, \\ &> 0. \end{aligned}$$

■

The Claim shows that x and y are separated by V . Thus along the line segment from \bar{x} to y there is a point v on the boundary of $V \cap P'$, since $y \in \text{int}(P' \cap V)$. v can be expressed as the convex combination of intersection points of the extreme rays of P' , and so $v \in \text{clconv}(P' \setminus \text{int}(C))$. Likewise, c is in P' and not in the interior of C , and so $c \in \text{clconv}(P' \setminus \text{int}(C))$. Since y is on the line segment connecting v and c , then $y \in \text{clconv}(P' \setminus \text{int}(C))$, which contradicts our initial supposition. \square

2.3 Strengthening the Intersection Cut

If some of the extreme rays of P' are contained in C , then the intersection cut is not in general sufficient to capture the convex hull of $P' \setminus C$. Negative step lengths λ_j^* can be used to derive stronger cuts. This was noted for the case of polyhedral S -free sets by Dey and Wolsey [32], and later for general S -free sets by Basu, Cornuéjols, and Zambelli [18] (see also [16]). We shall provide a general procedure for determining such step lengths.

A simple example of the issue is shown in Figure 1. Here $S \subset \mathbb{R}^2$ is given by the halfspace in $x_1 + x_2 \geq 1$. We let C be the (unique) maximal S -free set, $x_1 + x_2 \leq 1$. Now define the simplicial cone P' with inequalities $x_1 \geq 0$ and $x_2 \leq 0$. The apex of P' is at the origin, and the extreme ray directions are $r^{(1)} = (0, 1)$, $r^{(2)} = (0, -1)$. The intersection points with C are at $(1, 0)$ along $r^{(1)}$ and infinity along $r^{(2)}$. The intersection cut is given by $x_1 \geq 1$. The best cut possible from C , however is $x_1 + x_2 \geq 1$, i.e. the set S itself. To obtain this cut from P' one can use the original intersection point $(1, 0)$ together with $(0, 1)$, which can be obtained by taking a step of length -1 from the origin along $r^{(2)}$.

Changing say the k th step length λ_k to some new value λ'_k and holding all others fixed rotates the intersection cut about the axis defined by the $(n-1)$ fixed intersection points. This rotated cut can equivalently be generated by an intersection cut with C and a simplicial cone P'' that shares its apex and all extreme ray directions with P' except for the k th direction — call it $r_*^{(k)}$ — to which we assign infinite step length. Suppose the m th ray has finite intersection with C (the problem is infeasible if no such m exists). Then we have the parallel condition $r_*^{(k)} = \bar{x} + \lambda_m r^{(m)} - (\bar{x} + \lambda'_k r^{(k)})$, i.e. the direction $r_*^{(k)}$ is equal to the direction from the new intersection point (attained at negative step length) to one of the other intersection points. The rotated cut is valid if P'' is valid, i.e. $P'' \cap S = P' \cap S$. This can be guaranteed by ensuring $r_*^{(k)}$ is contained in the recession cone of C since by convexity of C any point in $P' \setminus P''$ would be in the interior of C hence outside S . Maximal rotation is given by $r_*^{(k)}$ parallel to an extreme ray of C .

Thus the strengthening procedure is to iterate over all extreme rays of P' with direction vectors strictly contained in the recession cone $\text{rec}(C)$. For each such ray $r^{(k)}$, we update the step length λ_k :

$$\lambda'_k := \max\{y | \lambda_m r^{(m)} - y r^{(k)} \in \text{rec}(C)\}. \quad (5)$$

In Section 5 we will show that this procedure can be performed efficiently for our proposed families of S -free sets.

2.4 Implementation of the Intersection Cut

An intersection cut for P requires the following:

1. A simplicial cone $P' \supseteq P$ with apex at \bar{x} .
2. An S -free set C containing \bar{x} in its interior.
3. For each extreme ray of P' , either the intersection with the boundary of C , or else proof that the ray is contained entirely in C .

Step 1 is satisfied using any n defining halfspaces of P with \bar{x} on their boundaries, i.e. setting P' to be a simplicial conic relaxation of P . This is possible provided P has at least one extreme point.

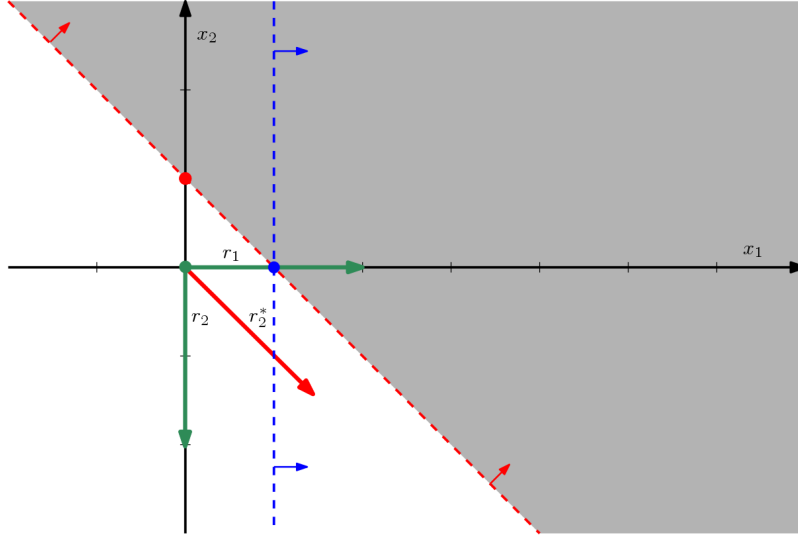


Figure 1: Example of cut tightening. In green, simplicial cone P' with rays r_1, r_2 ; origin marked with green dot. In grey, feasible set S , and the S -free set C is the complement of S . Blue dashes indicate the standard intersection cut; a blue dot marks the intersection point with $\text{bd}(C)$. The strengthened intersection cut is shown with red dashes; a red dot marks the intersection point obtained with a negative step length. The tightened extreme ray $r_2 \rightarrow r_2^*$ is shown in red.

Different choices of P' derived from P can affect the depth of the resulting cut. A natural approach is to select a cone corresponding to an optimal basic solution found from a LP relaxation, such as suggested by Gomory’s initial development of the cutting plane [41]. Since there may be many optimal solutions, the results are affected by the choice of LP solver. The dual simplex method is typically employed due to fast updating after applying a cut. Choices in the simplex pivoting rule can lead to substantially different results (e.g. the lexicographic rule [12, 83]). Other basic (possibly infeasible) solutions can also be used to generate intersection cuts; studies of optimizing over cut closures indicate the potential benefits of doing so (e.g. [14, 34]).

Step 2 shall be the focus of Section 4. Note there always exists an S -free set that can be used to separate \bar{x} . Since $\bar{x} \in \text{ext}(P)$, then $\bar{x} \notin \text{clconv}(S \cap P) \implies \bar{x} \notin S$. Since S is a closed set, then there exists a ball centered around \bar{x} that is S -free; for example, a lattice-free ball or cylinder is used in the original development of the intersection cut [9]. The S -free ball is a key notion used in Section 3.1.

Step 3 shall be the focus of Section 5. Note that a point precisely on the boundary is not necessary for a valid cut — points in the interior of C suffice. A simple way in practice to ensure numerical validity of the cut, for instance, is to take a sufficient step backwards from the boundary of C when generating intersection points. Computing valid points to generate a cut is computationally straightforward provided one can practically (e.g. in polynomial-time) determine membership in C .

Many cuts in mixed-integer linear programming can be interpreted as intersection cuts, as intersection cuts produce all nontrivial facets of the corner polyhedron [26]. For instance, split cuts are an important class of intersection cuts [2] due to their simplicity (derived from simple maximal

lattice-free sets) and practical effectiveness. Several papers [3, 28, 63, 64] have worked to extend the intersection cut via split cuts to mixed-integer conic optimization.

An important overarching consideration for cuts is cut pool management: using a subset of generated cuts when solving the relaxation in a given iteration (e.g. [1, 35, 58]). Judicial cut selection can improve convergence rate and numerical stability. Balas and Cornuejols [13] suggest managing a pool of intersection points derived from the intersection cut procedure with similar aims.

3 Oracle Ball Cuts

For a given point \bar{x} suppose we have an oracle providing the nonzero Euclidean distance $d(\bar{x}, S)$ between \bar{x} and the nearest point in S .

Remark. The ball $\mathcal{B}(\bar{x}, d(\bar{x}, S))$ is S -free.

Suppose P is a polytope. We can show that this S -free ball can be used to construct a pure cutting plane algorithm that will converge in the limit to the convex hull of $S \cap P$. Furthermore, an arbitrarily precise approximation of $\mathcal{B}(\bar{x}, d(\bar{x}, S))$ suffices to obtain an arbitrarily precise approximation of $\text{conv}(S \cap P)$ using the aforementioned algorithm. This is not as strong as convergence in finite time, which can be established for simpler problems (e.g. [41, 68]); such a guarantee is not possible here since $\text{conv}(S \cap P)$ may be nonlinear. Exact convergence, however, is not strictly necessary for effective practical implementation in branch-and-cut (e.g. split cuts [30]).

3.1 Separation

For any infeasible extreme point \bar{x} of P the intersection cut may be applied to $\mathcal{B}(\bar{x}, d(\bar{x}, S))$ to ensure separation (recall Proposition 2.4. The ball will not in general be a maximal S -free set, but together with the intersection cut it provides a simple, efficient (modulo the oracle call), and broadly applicable tool. Now suppose instead of generating a cut for $P' \setminus \mathcal{B}(\bar{x}, d(\bar{x}, S))$ we seek a cut $\alpha^T(x - \bar{x}) \geq \delta$ that separates \bar{x} from $P \setminus \mathcal{B}(\bar{x}, d(\bar{x}, S))$. The cut coefficients can be determined via the following master cut generation problem,

$$\begin{aligned} & \max \delta \\ (\mathbf{MC}) \quad & \text{s.t. } \alpha^T(x - \bar{x}) \geq \delta \quad \forall x \in \text{conv}(P \setminus \mathcal{B}(\bar{x}, d(\bar{x}, S))), \end{aligned} \tag{6a}$$

$$\|\alpha\|_2^2 \leq 1. \tag{6b}$$

The objective is to maximize the linear cut violation for the point \bar{x} . The cut normalization constraint (6b) is replaceable, for instance, with the 1-norm. Norm selection has been subject to extensive testing and discussion in mixed-integer programming (e.g. [36]), but we leave alternative formulations of **MC** out of scope of this initial proposal. In contrast to the intersection cut we subtract a ball over the entire polyhedron rather than a simplicial conic relaxation, which increases the computational burden of cut generation. Figure 2 demonstrates that one must separate over more than one nontrivial facet in general, and indeed the problem is NP-Hard [37]. The increased computational expense, however, provides us with strong cuts for which we are able to prove favourable convergence properties in Section 3.2.

One way to solve **MC** is to decompose in the fashion of Benders [20] by treating constraint (6a) with optimization. The convex constraint (6a) can be outer-approximated with linear cuts by

solving a subproblem: for a proposed candidate cut $\hat{\alpha}, \hat{\delta}$, we wish to find a point $\hat{x} \in \text{conv}(P \setminus \mathcal{B}(\hat{x}, d(\hat{x}, S)))$ for which $\hat{\alpha}^T(\hat{x} - \bar{x}) < \hat{\delta}$, or else certify that the cut is valid for equation (6a). This subproblem may be formulated as

$$z_{\text{SC}}^* := \max_x \|x - \bar{x}\|_2$$

$$\text{(SC)} \quad \text{s.t.} \quad \hat{\alpha}^T(x - \bar{x}) \leq \hat{\delta}, \tag{7a}$$

$$x \in P. \tag{7b}$$

If $z_{\text{SC}}^* \leq d(\hat{x}, S)$, then the cut $\hat{\alpha}, \hat{\delta}$ is valid. Otherwise, the corresponding optimal solution x^* (or a small perturbation if constraint (7b) is binding) can be used to add the cut $\alpha^T(\hat{x} - \bar{x}) \geq \delta$ to the master problem. If P is a rational polytope, then an optimal solution can be obtained in finite time using simplicial branch-and-bound [54].

The ellipsoid algorithm [43, 47] can be used to solve the master problem **MC** by solving a polynomial number of instances of **SC**, provided constraints (6a) and (6b) admit a strictly feasible point. The provision of strict feasibility is met if P is a polytope, as sufficiently small δ guarantees feasibility of any given α due to the bounded domain of x . Furthermore, to accommodate algorithms that can solve the master problem only to some fixed precision, there must be an adjustment for additive error $\lambda > 0$ where a smaller ball of radius $d(\bar{x}, S) - \lambda$ is used instead. This adjustment can also be used to accommodate imprecision in estimating the distance $d(\bar{x}, S)$, which may be irrational. As such, the proposed procedure can only separate points sufficiently far from S . This may be a necessary tradeoff with numerical methods due to the possibility of, say, the feasible set being a single irrational solution.

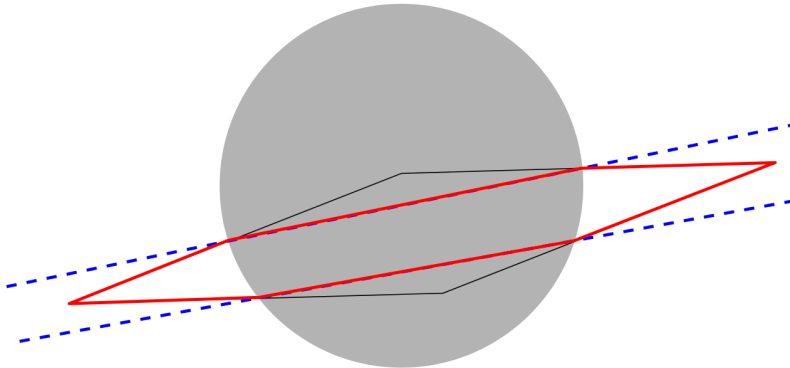


Figure 2: A parallelogram P minus a ball B . The convex hull of $P \setminus B$ shown in thick red lines; its nontrivial facets are described by the cuts with boundaries indicated by dotted blue lines.

3.2 Convergence of Cut Closures

Throughout this subsection we assume that P is a polytope. We follow closely the proof strategy of Theorem 3.6 in Averkov [8], which establishes convergence with respect to certain cuts given some structural assumptions on the structure of S . However, our result applies to closed sets S equipped with an oracle, which is a different domain of application than that of Averkov. Furthermore,

we allow for a cutting plane procedure with fixed numerical precision, where separation is only guaranteed over a ball with radius exceeding some minimum threshold $\lambda \geq 0$.

The Hausdorff distance between two sets X, Y , denoted $d_H(X, Y) := \max\{\sup_{x \in X} d(x, Y), \sup_{y \in Y} d(y, X)\}$, provides a natural way to describe convergence. An alternative definition of d_H is available using the notion of ϵ -fattening. The ϵ -fattening of a set X is $X_\epsilon := \cup_{x \in X} \mathcal{B}(x, \epsilon)$, and so $d_H(X, Y) = \inf\{\epsilon \geq 0 \mid X \succeq Y_\epsilon, Y \succeq X_\epsilon\}$.

Now relabel $P_0(\lambda) := P$, and define the rank k closure (see [24]) recursively as

$$P_{k+1}(\lambda) := \cap_{x \in \text{ext}(P_k(\lambda))} \text{conv}(P_k(\lambda) \setminus \mathcal{B}(x, \min\{d(x, S) - \lambda, 0\}))$$

Furthermore define the compact convex set $P_\infty(\lambda) := \cap_{k=0}^\infty P_k(\lambda)$, which is the infinite rank cut closure.

Two lemmas are used, with proofs that can be found in Schneider [73]. The first lemma gives us Hausdorff convergence in the sequence of cut closures [73, Lemma 1.8.2 & p. 69 Note 4].

Lemma 3.1. *Let $(C_k)_{k \in \mathbb{N}}$ be a sequence of nonempty compact sets in \mathbb{R}^n , and denote $C_\infty := \cap_{i=0}^\infty C_k$. If $C_k \supseteq C_{k+1} \forall k$ then $C_\infty = \lim_{k \rightarrow \infty} C_k$ and $\lim_{k \rightarrow \infty} d_H(C_k, C_\infty) = 0$.*

The second lemma [73, Lemma 1.4.6] ensures the existence of a ball cut that can separate an extreme point of a convex relaxation.

Lemma 3.2. *Let $C \subset \mathbb{R}^n$ be a closed, convex set and let $x \in C$. Then x is an extreme point of C iff for every open neighbourhood U around x there exists a hyperplane H defining the boundary of two (separate) halfspaces H^-, H^+ such that $x \in \text{int}(H^-), C \setminus U \in \text{int}(H^+)$.*

Theorem 3.3. $P_\infty(\lambda) \subseteq \text{conv}(P \cap S_\lambda)$.

Proof. By construction $P_\infty(\lambda) \subseteq P_0(\lambda) = P$, so it suffices to show that $\text{ext}(P_\infty(\lambda)) \in S_\lambda$. We shall do so by way of contradiction. Suppose there exists $\bar{x} \in \text{ext}(P_\infty(\lambda))$ such that $\bar{x} \notin S_\lambda$; observe that $\bar{x} \notin S_\lambda$ implies $d(\bar{x}, S) - \lambda > 0$. Then let U be an open ball of radius $r := (d(\bar{x}, S) - \lambda)/3$ centered at \bar{x} . By Lemma 3.2 there exist two opposite-facing halfspaces H^+, H^- such that $\bar{x} \in \text{int}(H^-)$ and $P_\infty(\lambda) \setminus U \in \text{int}(H^+)$. Since U is open and $P_\infty(\lambda) \cap H^-$ is in the interior of U , there exists sufficiently small $\epsilon > 0$ such that $(P_\infty(\lambda))_\epsilon \cap H^-$ is also contained in U . Now Lemma 3.1 gives us some rank k_0 for which we have the sandwich $(P_\infty(\lambda))_\epsilon \supseteq P_{k_0}(\lambda) \supseteq P_\infty(\lambda)$. Furthermore, since H^- separates an extreme point of $P_\infty(\lambda)$, it also separates an extreme point of the superset $P_{k_0}(\lambda)$. Thus there exists some extreme point $x_{k_0} \in \text{ext}(P_{k_0}(\lambda))$ in $P_{k_0}(\lambda) \cap H^- \subset U$, and so $d(x_{k_0}, \bar{x}) < r$. Thus we have

$$\begin{aligned} d(x_{k_0}, S) - \lambda &\geq d(\bar{x}, S) - d(x_{k_0}, \bar{x}) - \lambda \\ &> d(\bar{x}, S) - \lambda - r \\ &= 2r \end{aligned}$$

Since U has diameter $2r$, then $U \subset \mathcal{B}(x_{k_0}, d(x_{k_0}, S) - \lambda)$. Thus as H^+ is valid for $P_{k_0}(\lambda) \setminus U$, then H^+ is also valid for the nested set $P_{k_0}(\lambda) \setminus \mathcal{B}(x_{k_0}, d(x_{k_0}, S) - \lambda)$. However, $\bar{x} \in H^-$, which implies $\bar{x} \notin P_{k_0+1}(\lambda) \supseteq P_\infty(\lambda)$, giving us a contradiction. \square

A consequence of Theorem 3.3 is that the cutting plane procedure proposed in Section 3.1 can get arbitrarily close in Hausdorff distance to $\text{conv}(P \cap S)$ in finite time given sufficient numerical precision. For each extreme point \bar{x} of P_0 the cutting plane procedure can be applied to \bar{x} with the

ball $d(\bar{x}, S - \lambda)$, where λ is a parameter accounting for numerical tolerance in the solution to **MC**. This application of cuts yields $P_1(\lambda)$, and by recursive application any $P_k(\lambda)$ is attainable. Now suppose $P \cap S$ is nonempty and we seek a relaxation R that satisfies $d_H(R, \text{conv}(P \cap S)) \leq \epsilon$, where $\epsilon > 0$ is a precision parameter. Observe for any λ' such that $\epsilon > \lambda'$ we have $d_H(\text{conv}(P \cap S_{\lambda'}), \text{conv}(P \cap S)) < \epsilon$. Furthermore Theorem 3.3 gives us some r such that $d_H(P_r(\lambda'), \text{conv}(P \cap S_{\lambda'})) < \epsilon - \lambda'$. Hence, $P_r(\lambda')$, which is attainable by cutting plane algorithm (with precision satisfying tolerance λ'), satisfies our requirement for R . By similar argument, if $P \cap S$ is empty, then with sufficiently high numerical precision we can find a relaxation that is contained in an arbitrarily small neighbourhood. We note that if the 1-norm cuts are used instead of (6b) then, additionally, all computations can be assumed to take place over rationals.

4 Outer-Product-Free Sets

We shall follow the moment/sum-of-squares approach to polynomial optimization (see [50, 51]). Let d be the maximum degree of any monomial among the polynomials p_i . Let $m_r = [1, x_1, \dots, x_n, x_1x_2, \dots, x_n^2, \dots, x_n^r]$ be a vector of all monomials up to degree r . Any polynomial may be written in the form $p_i(x) = m_r^T A_i m_r$ (provided r is sufficiently large), where A_i is a symmetric matrix derived from coefficients of p_i . For instance,

$$x_1^2 + 2x_1x_2 + 2x_2 = \begin{bmatrix} 1 \\ x_1 \\ x_2 \end{bmatrix}^T \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ x_1 \\ x_2 \end{bmatrix}.$$

We can apply this transformation to **PO**:

$$\begin{aligned} & \min \langle A_0, X \rangle \\ (\mathbf{LPO}) \text{ s.t. } & \langle A_i, X \rangle \leq b_i, \quad i = 1, \dots, m, \end{aligned} \tag{8a}$$

$$X = m_r m_r^T. \tag{8b}$$

$A_i \in \mathbb{S}^{n \times n}$ are symmetric real matrices of data, and $X \in \mathbb{S}^{n \times n}$ is a symmetric real matrix of decision variables. The problem has linear objective function, linear constraints (8a), and nonlinear constraints (8b). This representation can be used to derive a semidefinite programming (SDP) relaxation, where $X = m m^T$ is replaced with the (symmetric) positive semidefinite constraint $X \succeq 0$. This SDP relaxation is called Shor's relaxation [75] and it is an exact relaxation when there is an optimal solution where $\text{rank}(X) = 1$ since the solution can be factorized to obtain an optimal solution vector for **PO**. In special cases (e.g. [50, 51, 56]) one can establish that there exists sufficiently large r to ensure an exact relaxation. However, there is a combinatorial explosion in the size of **LPO** (hence the size of any associated relaxation) with respect to r .

From **LPO** we have a natural definition of S : the set of symmetric matrices that are outer products: $\{xx^T : x \in \mathbb{R}^n\}$. Furthermore, P naturally corresponds to the linear constraints (8a). Accordingly, we shall study sets that are *outer-product-free*, where no matrix representable as a symmetric outer product is in the interior. S -free approach involves a vector space, so if $X \in \mathbb{S}^{n \times n}$, we consider the vectorized matrix $\text{vec}(X) \in \mathbb{R}^{n(n+1)/2}$, where entries from the upper triangular part of the matrix map to the vector in some order. Notions of the interior, convexity, and so forth are with respect to this vector space. For simplicity we shall drop the explicit vectorization where

obvious. Matrix theory will be used in the derivation of reciprocal step lengths β to determine intersection points.

Suppose we have an extreme point of a polyhedron P with spectral decomposition $\bar{X} := \sum_{i=1}^n \lambda_i d_i d_i^T$ and ordering $\lambda_1 \geq \dots \geq \lambda_n$. We shall study outer-product-free sets that strictly contain \bar{X} when it is not representable as a symmetric outer product.

4.1 Oracle Ball Cuts for Polynomial Optimization

Let k be the number of nonnegative eigenvalues of \bar{X} . Consider the following positive matrix approximation problem:

$$\begin{aligned} \min_Y \quad & \|\bar{X} - Y\| \\ (\mathbf{PMA}) \text{ s.t. } \quad & \text{rank}(Y) \leq r, \\ & Y \succeq 0. \end{aligned}$$

Here $\|\cdot\|$ is a unitarily invariant matrix norm such as the Frobenius norm, $\|\cdot\|_F$, which is the norm of singular values. Dax [29] proves the following:

Dax's Theorem. *For $1 \leq r \leq n-1$, an optimal solution to **PMA** is given by $\sum_{i=1}^{\min\{k,r\}} \lambda_i d_i d_i^T$.*

This can be considered an extension of an earlier result by Higham [44], which provided the solution for $r = n$. When \bar{X} is not negative semidefinite, the solution from Dax's theorem coincides with Eckart-Young-Mirsky [33, 60] solution to **PMA** without the positive semidefinite constraint. The optimal positive semidefinite approximant allows us to construct an outer-product-free ball:

$$\mathcal{B}_{\text{viol}}(\bar{X}) := \begin{cases} \mathcal{B}(\bar{X}, \|\bar{X}\|_F), & \bar{X} \text{ NSD}, \\ \mathcal{B}(\bar{X}, \|\bar{X} - \lambda_1 d_1 d_1^T\|_F), & \text{otherwise.} \end{cases}$$

Corollary 4.1. $\mathcal{B}_{\text{viol}}(\bar{X})$ is outer-product-free.

Proof. Setting $r = 1$ in Dax's Theorem, we see that the nearest symmetric outer product is either $\lambda_1 d_1 d_1^T$ if $\lambda_1 > 0$, or else the zeros matrix. \square

In the generic construction the violation ball is centered around \bar{X} since no further structure is assumed upon S when using an oracle. However, for **LPO** we can in certain cases use a simple geometric construction to make a bigger ball containing the original one. Given some ball with radius r , construct a ray v emanating from a point q on the boundary of the ball and passing through its centre. Consider a shifted ball with centre defined by taking a positive step length of s along the ray v and with q on its boundary.

Remark. If $s > r$ then the shifted ball contains the original ball. Algebraically we may write that for any $s > r$ we have $\mathcal{B}((s/r)X + (1-s/r)Q, s) \supset \mathcal{B}(X, r) \forall Q \in \mathbb{S}^{n \times n}$, or $\mathcal{B}(Q + (s/r)(X - Q), s) \supset \mathcal{B}(X, r) \forall Q \in \mathbb{S}^{n \times n}$.

Hence we can design a shifted violation ball by choosing a point on the boundary of $\mathcal{B}_{\text{viol}}$ and proceeding accordingly. Let us use the nearest symmetric outer product as the boundary point in our construction:

$$\mathcal{B}_{\text{shift}}(\bar{X}, s) := \begin{cases} \mathcal{B}(s\bar{X}/\|\bar{X}\|_F, s), & \bar{X} \text{ NSD}, \\ \mathcal{B}(\lambda_1 d_1 d_1^T + (s/\|\bar{X} - \lambda_1 d_1 d_1^T\|_F)(\bar{X} - \lambda_1 d_1 d_1^T), s), & \text{otherwise.} \end{cases}$$

Proposition 4.2. *Suppose \bar{X} is not a symmetric outer product. If $\lambda_2 \leq 0$ then $\mathcal{B}_{\text{shift}}(\bar{X}, \|\bar{X}\|_F + \epsilon)$ is outer-product-free and strictly contains $\mathcal{B}_{\text{viol}}(\bar{X})$ for $\epsilon > 0$. If $0 < \lambda_2 < \lambda_1$, then $\mathcal{B}_{\text{shift}}(\bar{X}, s)$ is outer-product-free and strictly contains $\mathcal{B}_{\text{viol}}(\bar{X})$ for $\lambda_2 < s \leq \lambda_1$.*

Proof. Strict containment is assured by construction, so it suffices to show that $\mathcal{B}_{\text{shift}}$ is outer-product-free.

First suppose \bar{X} is negative semidefinite,

$$\begin{aligned} \mathcal{B}_{\text{shift}}(\bar{X}, \|\bar{X}\|_F + \epsilon) &= \mathcal{B}((\|\bar{X}\|_F + \epsilon)\bar{X}/\|\bar{X}\|_F, \|\bar{X}\|_F + \epsilon), \\ &= \mathcal{B}((1 + \epsilon/\|\bar{X}\|_F)\bar{X}, \|\bar{X}\|_F + \epsilon). \end{aligned}$$

$(1 + \epsilon/\|\bar{X}\|_F)$ is negative semidefinite due to our negative semidefinite assumption on \bar{X} , so from Dax's theorem we know the nearest outer-product is the all zeros matrix. Hence for $\mathcal{B}_{\text{shift}}$ to be outer-product-free, its radius can be no more than the Frobenius norm of its centre, $(1 + \epsilon/\|\bar{X}\|_F)$, which by observation is indeed the case.

Now suppose \bar{X} has at least one positive eigenvalue,

$$\begin{aligned} \mathcal{B}_{\text{shift}}(\bar{X}, s) &= \mathcal{B}(\lambda_1 d_1 d_1^T + (s/\|\bar{X} - \lambda_1 d_1 d_1^T\|_F)(\bar{X} - \lambda_1 d_1 d_1^T), s), \\ &= \mathcal{B}(\lambda_1 d_1 d_1^T + (s/\|\sum_{i=2}^n \lambda_i d_i d_i^T\|_F) \sum_{i=2}^n \lambda_i d_i d_i^T, s). \end{aligned}$$

If $\lambda_2 \leq 0$ then the nearest outer product by Dax's theorem is $\lambda_1 d_1 d_1^T$. The maximum radius outer-product-free ball is thus $\|(s/\|\sum_{i=2}^n \lambda_i d_i d_i^T\|_F) \sum_{i=2}^n \lambda_i d_i d_i^T\|_F = s$, and so $\mathcal{B}_{\text{shift}}(\|\bar{X}\|_F + \epsilon)$ is outer-product-free for all $\epsilon > 0$.

If $0 < \lambda_2 < \lambda_1$, then by Dax's theorem the nearest outer product is $\lambda_1 d_1 d_1^T$ iff

$$\begin{aligned} \lambda_1 &\geq (s/\|\sum_{i=2}^n \lambda_i d_i d_i^T\|_F) \lambda_2, \\ \implies s &\leq \|\sum_{i=2}^n \lambda_i d_i d_i^T\|_F \lambda_1 / \lambda_2. \end{aligned}$$

This condition is satisfied for $\lambda_2 < s \leq \lambda_1$, and so the nearest outer product to the centre of the proposed shifted ball is $\lambda_1 d_1 d_1^T$. This gives us a maximum radius of

$$\|(s/\|\sum_{i=2}^n \lambda_i d_i d_i^T\|_F) \sum_{i=2}^n \lambda_i d_i d_i^T\|_F = s.$$

□

4.2 Maximal Outer-Product-Free Sets

We shall establish that maximal outer-product-free sets with full dimension are cones. Then, such cones will be classified in terms of the coefficient matrices corresponding to their supports. This classification will lead to several families with which we can perform polynomial-time separation.

Lemma 4.3. *Let $C \subseteq \mathbb{R}^n$ be a convex set. Every ray emanating from the origin and contained in $\text{cone}(C)$ passes through a point in C that is not the origin.*

Proof. Consider a ray r emanating from the origin and in $\text{cone}(C)$. Any point x along r that is not the origin has conic representation $\sum_{i=1}^k \lambda_i c_i$ where $k \geq 1, \lambda > 0, c_i \in C \forall i$. Consequently, r passes through the point $x/(\sum_{i=1}^k \lambda_i)$, which is a convex combination of points in and therefore itself an element of C . \square

Lemma 4.4. *Let $C \subseteq \mathbb{R}^n$ be a convex set with full dimension. Every ray emanating from the origin and contained in $\text{cone}(C)$ either intersects with the interior of C or is contained in the boundary of $\text{cone}(C)$.*

Proof. Suppose not. Then there exists a ray r emanating from the origin with direction $d \in \mathbb{R}^n$ that is contained in the interior of $\text{cone}(C)$ but does not intersect with $\text{int}(C)$. Furthermore since r is in the interior of $\text{cone}(C)$, there exists $\epsilon > 0$ such that $(d + \epsilon p)t \in \text{cone}(C)$ for all $p \in \mathbb{R}^n, t \geq 0$. However, Lemma 4.3 implies r is tangent to the boundary of C , and so there exists some \hat{p} such that $(d + \epsilon \hat{p})t$ is separated by a hyperplane supporting C for all $t > 0$. Hence the ray emanating from the origin in the direction $(d + \epsilon \hat{p})$ can only intersect with C at the origin; by Lemma 4.3 this implies the ray is not contained in $\text{cone}(C)$. \square

Theorem 4.5. *Let $C \subset \mathbb{S}^{n \times n}$ be an outer-product-free set with full dimension. Then $\text{clcone}(C)$ is outer-product-free.*

Proof. Suppose $\text{clcone}(C)$ is not outer-product-free; since it is closed and convex, there must exist $d \in \mathbb{R}^n$ such that dd^T is in its interior. If d is the zeros vector, then $\text{int}(C)$ also contains the origin, which contradicts the condition that C be outer-product-free. Otherwise the ray r emanating from the origin with nonzero direction dd^T is entirely contained in $\text{clcone}(C)$ and passes through its interior. By convexity the interior of $\text{cone}(C)$ is the same as the interior of its closure, so r is also passes through the interior of $\text{cone}(C)$. By Lemma 4.4, r intersects with the interior of C . But every point along r is an outer-product, which again implies that C is not outer-product-free. \square

Corollary 4.6. *Every maximal outer-product-free set with full dimension is a convex cone.*

Proof. Follows directly from Theorem 4.5. \square

Definition 4.7. A supporting halfspace of a set S contains S and shares its boundary with a supporting halfspace of S . Thus it is defined by some $a, b \in \mathbb{R}^n \times \mathbb{R}$ such that $a^T x \leq b \forall x \in S$ and there exists $\hat{x} \in S$ such that $a^T \hat{x} = b$.

Lemma 4.8. *Let C be a maximal outer-product-free set with full dimension. Any supporting halfspace of C is of the form $\langle A, X \rangle \geq 0$ for $A \in \mathbb{S}^{n \times n}$.*

Proof. From Corollary 4.6 we have that C is a convex cone. A generic way of writing a halfspace is $\langle A, X \rangle \geq b$. If $b \neq 0$, then there exists some nonzero X^* at the boundary of the cone such that $\langle A, X^* \rangle = b$. However, by property of a cone we require $\langle \alpha A, X^* \rangle \geq b$ for all $\alpha \geq 0$, which is impossible. \square

From Lemma 4.8 we may thus characterize a maximal outer-product-free set as $C = \{X \in \mathbb{S}^{n \times n} \mid \langle A_i, X \rangle \geq 0 \forall i \in I\}$, where I is an index set that is not necessarily finite. It will be useful to classify each supporting halfspace in terms of its coefficient matrix: A is either positive semidefinite, negative semidefinite, or indefinite.

Theorem 4.9. *The halfspace $\langle A, X \rangle \geq 0$ is maximal outer-product-free iff A is negative semidefinite.*

Proof. If A is positive semidefinite or indefinite, then it has a strictly positive eigenvalue with corresponding eigenvector d . Then $\langle A, dd^T \rangle > 0$, and so the halfspace is not outer-product-free.

If A is negative semidefinite we have $\langle A, dd^T \rangle = d^T A d \leq 0 \forall d \in \mathbb{R}^n$, so the halfspace is outer-product-free. For maximality, suppose the halfspace is strictly contained in another outer-product-free set \bar{C} . Then there must exist some interior point in \bar{C} , \bar{X} such that $\langle A, \bar{X} \rangle < 0$. However, $\langle A, (-\bar{X}) \rangle > 0$, and so the zeros matrix is interior to \bar{C} since it lies between \bar{X} and $-\bar{X}$. Thus \bar{C} cannot be outer-product-free. \square

Corollary 4.10. *Let C be a maximal outer-product-free set with full dimension with supporting halfspaces indexed by the set I . If there exists $i \in I$ such that A_i is negative semidefinite, then C is exactly the halfspace $\langle A_i, X \rangle \geq 0$.*

Proof. Suppose C is contained in the halfspace $\langle A_i, X \rangle \geq 0$ with A_i NSD. By Theorem 4.9 the halfspace is outer-product-free, and so C is maximal only if it is the supporting halfspace itself. \square

Definition 4.11. A 2×2 PSD cone is of the form $\{X \in \mathbb{S}^{n \times n} | X_{[i,j]} \succeq 0\}$, with $1 \leq i \neq j \leq n$.

Remark. Every 2×2 PSD cone is a closed, convex set. Furthermore, all its supporting halfspaces are positive semidefinite.

Theorem 4.12. *Every 2×2 PSD cone is maximal outer-product-free.*

Proof. Every real, symmetric outer product has rank one and is PSD, and so all its 2×2 principal submatrices are PSD and have rank one. Thus every such outer product is on the boundary of all 2×2 PSD cones. Every 2×2 PSD cone, being closed and convex, is therefore outer-product-free.

Now by way of contradiction suppose for some (i, j) the corresponding 2×2 PSD cone is not maximal outer-product-free. Then it is contained in an outer-product-free set \bar{C} . Furthermore there must exist $\bar{X} \in \bar{C}$ such that $\bar{X}_{[i,j]}$ is not positive semidefinite. Then we may write a spectral decomposition $\bar{X}_{[i,j]} := \lambda_1 d_1 d_1^T + \lambda_2 d_2 d_2^T$ where λ_2 is strictly negative. We shall now construct a matrix Y in the interior of the 2×2 PSD cone, and hence in the interior of \bar{C} . Choose some $\epsilon > 0$ and set $Y_{[i,j]} := (|\lambda_1| + \epsilon) d_1 d_1^T + |\lambda_2| d_2 d_2^T$. Furthermore for all other entries of Y , set $Y_{k,\ell} = -\bar{X}_{k,\ell}$. By construction $Y_{[i,j]}$ is positive definite and therefore in the interior of \bar{C} . Now let $Z := (\bar{X} + Y)/2$ be the midpoint between \bar{X} and Y . Then we have $Z = zz^T$, where the (i, j) entries of z are equal to the (i, j) entries of $\sqrt{|\lambda_1| + \epsilon} d_1$ and all other entries of z are zero. Thus zz^T is the convex combination of $\bar{X} \in \bar{C}$ and $Y \in \text{int}(\bar{C})$, and so \bar{C} is not outer-product-free. \square

We can also demonstrate existence of other maximal outer-product-free sets that have supporting halfspaces with PSD coefficient matrices. First let us characterize all maximal outer-product-free sets containing the cone of positive semidefinite matrices, $\mathbb{S}^{n \times n}$. Our approach involves Weyl's inequality [81]. Let A, B be Hermitian matrices and define $C := A + B$. Let the eigenvalues of A, B, C be μ, ν, ρ respectively, with orderings $\mu_1 \leq \dots \leq \mu_n, \nu_1 \leq \dots \leq \nu_n, \rho_1 \leq \dots \leq \rho_n$.

Weyl's Inequality. *For $i = 1, \dots, n$ and $j + k - n \leq i \leq r + s - 1$, we have*

$$\nu_j + \rho_k \leq \mu_i \leq \nu_r + \rho_s.$$

Lemma 4.13. *Let $\bar{X} \in \mathbb{S}^{n \times n}$ be a symmetric matrix with k nonnegative eigenvalues. $\text{conv}(\bar{X} \cup \mathbb{S}_+^{n \times n})$ is outer-product-free iff $k \geq 2$.*

Proof. We shall write a spectral decomposition $\bar{X} = \sum_{i=1}^n \lambda_i d_i d_i^T$ with ordering $\lambda_1 \geq \dots \geq \lambda_n$. The outer-product-free condition is equivalent to the condition that there does not exist $c \in \mathbb{R}^n$ and radius $\epsilon > 0$ such that $\mathcal{B}(cc^T, \epsilon) \in \text{conv}(\bar{X} \cup \mathbb{S}_+^{n \times n})$. The ball condition can be restated as follows: for each $Q \in \mathbb{S}^{n \times n}$ with bounded Frobenius norm $\|Q\|_F \leq 1$ there exists $\alpha \in [0, 1], R \in \mathbb{S}_+^{n \times n}$ so that $cc^T + \epsilon Q = \alpha \bar{X} + (1 - \alpha)R$, or

$$cc^T + \epsilon Q - \alpha \bar{X} \succeq 0.$$

We will show the ball condition holds for $k \leq 1$, and show that no such construction is possible for $k \geq 2$.

Suppose $k \leq 1$. We shall demonstrate that $\beta d_1 d_1^T$ is in the interior of $\text{conv}(\bar{X} \cup \mathbb{S}_+^{n \times n})$, for $\beta > |\lambda_1|$. By construction, we have that $\beta d_1 d_1^T - \alpha \bar{X}$ is a strictly positive definite matrix. From Weyl's inequality we have for any symmetric A, B that the minimum eigenvalue of the sum is bounded as follows: $\lambda_{\min}(A + B) \geq \lambda_{\min}(A) + \lambda_{\min}(B)$. Setting ϵ to the minimum eigenvalue of $\beta d_1 d_1^T - \alpha \bar{X}$ gives the desired result:

$$\begin{aligned} & \lambda_{\min}(\beta d_1 d_1^T + \epsilon Q - \alpha \bar{X}), \\ & \geq \lambda_{\min}(\beta d_1 d_1^T - \alpha \bar{X}) + \lambda_{\min}(\epsilon Q), \\ & \geq \lambda_{\min}(\beta d_1 d_1^T - \alpha \bar{X}) - \epsilon, \\ & \geq 0. \end{aligned}$$

Note that we have relied on the fact that the Frobenius norm of Q is bounded by 1, and so each singular value (thus the magnitude of any eigenvalue) is at most 1.

Now suppose $k \geq 2$. Consider some $c \in \mathbb{R}^n, \epsilon > 0$. Let C^\perp be the orthogonal complement of c , and let $G = \text{span}\{d_1, d_2\}$. Then, using a standard dimension argument from linear algebra (e.g. [65, p. 48]), we can show the intersection of these sets is nonempty:

$$\begin{aligned} \dim(C^\perp \cap G) &= \dim(C^\perp) + \dim(G) - \dim(C^\perp + G), \\ &\geq (n - 1) + 2 - n, \\ &\geq 1. \end{aligned}$$

Now consider some nonzero $v \in C^\perp \cap G$. Setting $Q = -vv^T / \|v\|_2^2$ We have

$$\begin{aligned} & v^T (cc^T + \epsilon Q - \alpha \bar{X}) v, \\ &= v^T (-\epsilon vv^T / \|v\|_2^2 - \alpha \bar{X}) v, \\ &\leq v^T (-\epsilon vv^T) v / \|v\|_2^2 < 0. \end{aligned}$$

Thus in this case no such ball $\mathcal{B}(cc^T, \epsilon)$ can be in $\text{conv}(\bar{X} \cup \mathbb{S}_+^{n \times n})$, and so the convex hull is outer-product-free. \square

As a consequence of Lemma 4.13 we can characterize all outer-product-free sets in $\mathbb{S}^{2 \times 2}$.

Corollary 4.14. $\mathbb{S}^{n \times n}$ is maximal outer-product-free iff $n = 2$.

Proof. Follows immediately from Lemma 4.13. \square

Lemma 4.15. *In $\mathbb{S}^{2 \times 2}$ the cone of positive semidefinite matrices is the unique maximal outer-product-free set containing at least one positive semidefinite matrix in its interior.*

Proof. From Corollary 4.14 we have that the cone of PSD matrices is maximal for $n = 2$. Hence, if there exists a maximal outer-product-free set containing a PSD matrix in its interior, it consequently contains a boundary point of $\mathbb{S}_+^{n \times n}$ — otherwise, it is a subset of the PSD cone. However, every boundary point of the PSD cone is a symmetric, real outer product for $n = 2$. \square

Theorem 4.16. *In $\mathbb{S}^{2 \times 2}$ every maximal outer-product-free set of full dimension is either the cone of positive semidefinite matrices or a halfspace of the form $\langle A, X \rangle \geq 0$, where P is a symmetric negative semidefinite matrix.*

Proof. From Lemma 4.15, we have that every maximal outer-product-free set is either the cone of positive semidefinite matrices or it does not contain a PSD matrix in its interior. Now suppose $C \in \mathbb{S}^{n \times n}$ is a maximal outer-product-free set that is not the cone of positive semidefinite matrices. C is thus a closed, convex set that does not share an interior with $\mathbb{S}^{2 \times 2}$. Then by separating hyperplane theorem there exists a supporting hyperplane of $\mathbb{S}^{2 \times 2}$, which by Lemma 4.8 and Lemma 4.15 is of the form $\langle A, X \rangle = 0$, such that C is contained in the halfspace $\langle A, X \rangle \geq 0$. But if A has a positive eigenvalue then the halfspace includes at least one PSD matrix; thus so to maintain separation A is necessarily negative semidefinite. Furthermore, for any negative semidefinite A the halfspace $\langle A, X \rangle \geq 0$ is outer-product-free by Theorem 4.9 so C must be the halfspace itself in order to be maximal outer-product-free. \square

We can show that for $n \geq 3$ there exist other types of maximal outer-product-free sets that are composed entirely of supporting halfspaces with PSD coefficient matrices, as well as maximal outer-product-free sets at least one supporting halfspace that has indefinite coefficient matrix. This can be done by constructing an appropriate outer-product-free set and applying the following result from Conforti et al. [25] (the proof of which assumes the axiom of choice):

CCDLM Theorem. *Every S -free set is contained in a maximal S -free set.*

Their definition of S -free set includes a further requirement that S does not contain the origin, however for our purposes this is a nonrestrictive assumption as affine shifts can be applied as needed.

Proposition 4.17. *For $n \geq 3$ there exists a maximal outer-product-free set $C \subset \mathbb{S}^{n \times n}$ with full dimension such that the supporting halfspaces of C all have PSD coefficient matrices and C is not a 2×2 PSD cone.*

Proof. Define in $\mathbb{S}^{n \times n}$ the matrix $\bar{X} := I - \mathbf{1}\mathbf{1}^T$, where $\mathbf{1}$ is the vector of all ones. Observe $\bar{X}\mathbf{1} = (1 - n)\mathbf{1}$, and so $(1 - n)$ is an eigenvalue. Furthermore, $|\bar{X} - (1)I| = |-\mathbf{1}\mathbf{1}^T| = 0$, and so 1 is an eigenvalue. Any eigenvector d corresponding to the eigenvalue 1 is of the form $(I - \mathbf{1}\mathbf{1}^T)d = d$, and so $\mathbf{1}\mathbf{1}^T d = 0$, which implies the eigenvalue -1 has multiplicity $n - 1$. Then for $n \geq 3$, we have by Lemma 4.13 that $Y := \text{conv}(\bar{X} \cup \mathbb{S}_+^{n \times n})$ is outer-product-free. By the CCDLM Theorem Y is contained in some maximal outer-product-free set C , and since C contains the PSD cone it cannot have a supporting halfspace with indefinite or negative semidefinite coefficient matrix by Lemma 4.8. Furthermore, all the 2×2 principal submatrices of \bar{X} are indefinite, and so C is not a 2×2 PSD cone. \square

Proposition 4.18. *For $n \geq 3$ there exists a maximal outer-product-free set $C \subset \mathbb{S}^{n \times n}$ with full dimension such at least one supporting halfspace of C is of the form $\langle A, X \rangle \geq 0$, where A is an indefinite symmetric coefficient matrix.*

Proof. We shall construct an outer-product-free set \bar{C} with full dimension containing both a positive definite and negative definite matrix. Let Y be the diagonal matrix $Y := \text{diag}(-1, \dots, -1, -2)$, and let ℓ be the line defined by $I + \alpha Y, \alpha \in \mathbb{R}$. The eigenvalues at a point along the line parameterized by α are the diagonal entries $(1 - \alpha, \dots, 1 - \alpha, 1 - 2\alpha)$. By Dax's theorem the Euclidean distance to the nearest real, symmetric outer product is

$$\begin{aligned} & \sqrt{n-1}(1-\alpha), & \alpha \leq 0, \\ & \sqrt{(n-2)(1-\alpha)^2 + (1-2\alpha)^2}, & 1 > \alpha > 0, \\ & \sqrt{(n-1)(1-\alpha)^2 + (1-2\alpha)^2}, & \alpha \geq 1. \end{aligned}$$

As each segment is a convex function with respect to α , the minimum distance to an outer product along line ℓ can be calculated by setting derivatives to zero or taking extreme values of the interval, yielding the following minima:

$$\begin{aligned} & \sqrt{n-1}, & \alpha \leq 0, \\ & \sqrt{(n-2)/(n+2)}, & 1 > \alpha > 0, \\ & 1, & \alpha \geq 1. \end{aligned}$$

The minimum radius along ℓ is therefore $\sqrt{(n-2)/(n+2)}$, and so the full-dimensional cylinder \bar{C} with ℓ as its axis and radius $\sqrt{(n-2)/(n+2)}$ is outer-product-free. By CCDLM theorem, \bar{C} is contained in some maximal outer-product free set C . Lemma 4.8 tells us that the supporting halfspaces are all of the form $\langle A, X \rangle \leq 0$, and C contains the identity matrix, so no such halfspace can have a negative semidefinite coefficient matrix. Furthermore, if all supporting halfspaces were to have positive semidefinite coefficient matrices, then C would contain the PSD cone. However, C contains negative definite matrices, for instance $\text{diag}(-1, \dots, -1, -3)$, and so by Lemma 4.13 it cannot contain the PSD cone and be maximal outer-product-free. Hence at least one supporting halfspace of C must have indefinite (symmetric) coefficient matrix. \square

5 Intersection Cuts for Polynomial Optimization

In this section we discuss the implementation of Step 3 of the intersection cut as described in Section 2.4. In particular, given a simplicial cone P' with apex \bar{X} , we discuss how to select appropriate outer-product-free sets among those given in Section 4 and how to generate the step lengths λ .

5.1 Oracle Ball Cuts

The violation ball $\mathcal{B}_{\text{viol}}(\bar{X})$ and its extension $\mathcal{B}_{\text{shift}}(\bar{X}, s)$ by construction apply to any \bar{X} that is not a symmetric, real outer-product. Calculation of the radius and centre of either ball can be done

using the spectral decomposition of \bar{X} , as discussed in Section 4.1. For $\mathcal{B}_{\text{viol}}$, the step lengths λ are all equal to the radius of the ball. The extended ball $\mathcal{B}_{\text{shift}}$ will not in general have \bar{X} as its centre, and requires some adjustment. Given a ball $\mathcal{B}(x, r)$ and extreme ray $y + \alpha d, \alpha \geq 0$ that is emanating from a point y inside the ball, the intersection with the boundary occurs when the following holds:

$$\begin{aligned} d(x, y + \alpha d) &= r, \\ \implies \sum_i (x_i - y_i - \alpha d_i)^2 &= r^2. \end{aligned}$$

Taking the positive root of the quadratic equation with respect to α gives the desired step length.

5.2 2×2 PSD Cone

Some, but not all indefinite matrices lie strictly inside a 2×2 PSD cone. Furthermore, the following proposition of Chen, Atamturk and Oren [23], ensures that every positive semidefinite matrix with rank greater than one is in a 2×2 cone:

CAO Proposition. *For $n > 1$ a nonzero Hermitian positive semidefinite $n \times n$ matrix X has rank one iff all of its 2×2 principal minors are zero.*

Selecting appropriate 2×2 submatrices is straightforward: enumerate over all 2×2 submatrices and check for positive definiteness, i.e. $X_{ii}, X_{jj} > 0, X_{ii}X_{jj} > X_{ij}^2$. For a given (i, j) -cone, intersections can be found by taking the 2×2 principal submatrices $\bar{X}_{[i,j]}, D_{[i,j]}^{(k)}$ respectively corresponding to \bar{X} and some extreme ray direction $D^{(k)}$.

First suppose $D_{[i,j]}^{(k)}$ is not positive semidefinite. Then we seek the step length $\lambda_k \geq 0$ such that $\bar{X}_{[i,j]} + \lambda_k D_{[i,j]}^{(k)}$ lies on the boundary of the 2×2 cone, i.e. the minimum eigenvalue is zero. Now for a symmetric matrix $\begin{bmatrix} a & b \\ b & c \end{bmatrix}$ the minimum eigenvalue can be expressed as

$$(a + c - \sqrt{a^2 - 2ac + 4b^2 + c^2})/2.$$

The eigenvalue is zero when $ac = b^2, a + c \geq 0$. Applying this to $\bar{X}_{[i,j]} + \lambda_k D_{[i,j]}^{(k)}$, we have

$$((D_{ij}^{(k)})^2 - D_{ii}^{(k)} D_{jj}^{(k)}) \lambda_k^2 + (2D_{ij}^{(k)} X_{ij} - D_{ii}^{(k)} X_{jj} - D_{jj}^{(k)} X_{ii}) \lambda_k + X_{ij}^2 - X_{ii} X_{jj} = 0.$$

The desired step length is given by the greater root of this quadratic equation with respect to λ_k (the lesser root sets the maximum eigenvalue to zero).

Now suppose $D_{[i,j]}^{(k)}$ is positive semidefinite. Then $\bar{X}_{[i,j]} + \lambda_k D_{[i,j]}^{(k)}$ is positive semidefinite for all nonnegative λ_k , giving us an intersection at infinity; thus we can apply the strengthening procedure outlined in Section 2.3. Let m be the index of an extreme ray of P' with finite intersection. Specializing equation 5 we have:

$$\lambda'_k := \max\{y | \lambda_m D^{(m)} - y D^{(k)} \succeq 0\}$$

Table 1: Proposed Cuts

Cut Name	S -free set	Separation Condition
2×2 Cut	$X_{[i,j]} \succeq 0$	$\bar{X}_{[i,j]} \succ 0$
Outer Approximation Cut	$c^T X c \leq 0$	\bar{X} NSD or indefinite
Oracle Ball Cut	$\mathcal{B}_{\text{viol}}$	\bar{X} not an outer product
Shifted Oracle Ball Cut	$\mathcal{B}_{\text{shift}}$	\bar{X} not an outer product

Note that λ'_k is bounded since $D^{(k)}$ is strictly positive definite. When the PSD constraint is binding we have $\lambda_{\min}(\lambda_m D^{(m)} - y D^{(k)}) = 0$. Setting the 2×2 determinant to zero yields the necessary condition

$$(\lambda_m D_{11}^{(m)} - y D_{11}^{(k)})(\lambda_m D_{22}^{(m)} - y D_{22}^{(k)}) = (\lambda_m D_{12}^{(m)} - y D_{12}^{(k)})^2$$

This is a quadratic equation in y with at least one solution guaranteed by definiteness of $D^{(k)}$.

5.3 Outer-Approximation Cuts

The maximal outer-product-free sets described by Theorem 4.9 are halfspaces, and so the best possible cuts that can be derived from these are of the form $\langle A, X \rangle \leq 0$, where A is NSD. However, observe that if A has rank $k > 1$, then the cut is of the form $\sum_{i=1}^k \lambda_i d_i^T X d_i \leq 0$, where each λ_i is a negative eigenvalue. Then the inequality is implied by and thus weaker than the individual inequalities of the form $\lambda_i d_i^T X d_i \leq 0$. These individual inequalities are valid as they are necessary for the positive semidefinite condition on X . Indeed, imposing all cuts of the form $c^T X c \leq 0$ is equivalent to enforcing the convex constraint $X \succeq 0$, and so the halfspaces described by Theorem 4.9 characterize the outer-approximation cuts of the SDP relaxation to **LPO**. Therefore separation is only possible if the given point is NSD or indefinite. A natural approach to separation that we shall adopt is to use all negative eigenvectors of a given extreme point of P as cut coefficient vectors. This is a well-studied procedure for semidefinite programming problems [49, 69, 72, 74].

5.4 Summary of Cuts

The proposed cuts are summarized in Table 1. Since the 2×2 cut will separate any rank two or greater PSD matrix and the outer approximation cuts will separate NSD or indefinite matrices, then the two families of cuts can be applied in tandem for global separation. $\mathcal{B}_{\text{shift}}$ provides a stronger cut than $\mathcal{B}_{\text{viol}}$ and can be used alone or in combination with the other cuts.

6 Numerical Examples

We begin with a simple example in $\mathbb{S}^{2 \times 2}$, a case that is fully understood and can be represented directly in three dimensions. Consider the following polynomial optimization problem:

$$\begin{aligned}
& \min x_1 x_2 \\
& \text{s.t.} \quad -x_1^2 - x_2^2 + x_1 x_2 \leq -2, \\
& \quad \quad -x_1^2 - x_2^2 - x_1 x_2 \leq -2, \\
& \quad \quad -x_1^2 + x_2^2 - x_1 x_2 \leq 0.
\end{aligned}$$

An **LPO** representation is

$$\begin{aligned}
& \min X_{12} \\
& \text{s.t.} \quad -X_{11} - X_{22} + X_{12} \leq -2, & (10a) \\
& \quad \quad -X_{11} - X_{22} - X_{12} \leq -2, & (10b) \\
& \quad \quad -X_{11} + X_{22} - X_{12} \leq 0, & (10c) \\
& \quad \quad X = xx^T. & (10d) \\
& & (10e)
\end{aligned}$$

Dropping the outer product constraint (10d) results in a linear program — indeed, by construction the linear constraints describe a simplicial cone. The optimal solution \bar{X} to this linear relaxation is at the apex of the simplicial cone,

$$\bar{X} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}.$$

The extreme rays emanating from \bar{X} have the following directions:

$$D_1 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, D_2 = \begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix}, D_3 = \begin{bmatrix} 1 & -1 \\ -1 & 0 \end{bmatrix}.$$

D_1 is determined by (10a) and (10b); D_2 by (10a) and (10c); D_3 by (10b) and (10c).

2×2 cut. The three intersection points are of the form $\bar{X} + \alpha_i D_i$, where α is a vector of step sizes. The intersection with the boundary of the cone of is obtained by setting $\alpha_1 = 1, \alpha_2 = \alpha_3 = \phi$, where $\phi := \frac{1+\sqrt{5}}{2}$ is the golden ratio. The intersection cut passing through these points is given by $PX \geq 1$, where

$$P \cong \begin{bmatrix} 0.5 & 0.2236 \\ 0.2236 & 0.0264 \end{bmatrix}.$$

Outer Approximation Cut As the apex is strictly positive definite, no outer approximation can separate it.

Oracle Ball Cut Both eigenvalues of \bar{X} are equal to one, and so the radius of the ball and every step length is 1. Hence the cut is strictly dominated by the 2×2 cut. From Proposition 4.2 we have equal eigenvalues, and so the shifting has no effect.

7 Conclusions

In this paper we introduced cuts for the generic set $S \cap P$, where for the closed set S we have an oracle that provides the distance from a point to the nearest point in S . This oracle was then used to construct a convergent cutting plane algorithm that can produce arbitrarily close approximations to $\text{conv}(S \cap P)$ in finite time. This algorithm relied on a potentially computationally expensive cut generation procedure, and we leave as an open question whether the closure over ball cuts can attain similarly favourable convergence results.

This paper also provided cuts for the special case of polynomial optimization, where S is the set of real, symmetric outer products. These cuts are based on a new theory of maximal outer-product-free sets. Our results include a full characterization of such sets over 2×2 matrices, as well as a link between a family of maximal outer-product-free sets and outer-approximation cuts for semidefinite programming. Propositions 4.17 and 4.18 some open avenues that may be worth pursuing. Future work will concern empirical testing of these cuts on polynomial optimization instances.

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